LA-UR-19-29312

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Intended for:	Report
Issued:	2019-09-16

EVPSC modeling of 316 stainless steel with and without observed phase transformation.

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The following is a description of modeling the constitutive behavior of the transforming and non-transforming 316 stainless steel measured in-situ at APS. Details of the elasto-viscoplastic self-consistent (EVPSC) polycrystal deformation model are described in the literature [1,2] and only the salient information is given here. The EVPSC model is a general rate-sensitive self-consistent polycrystal plasticity model valid at arbitrary large deformations. The homogenizing method used is the self-consistent approach, originally proposed by Kröner [3], assuming that each grain is an ellipsoidal inclusion embedded in an infinite homogeneous equivalent medium (HEM), where the interaction is determined using Eshelby's solution [4].The hardening behavior is described by a Voce type strain hardening law, and the phase transformation uses a strain energy criterion for choosing a single daughter grain for each parent grain that reaches a critical value of the Von Mises equivalent strain. The orientation relationship between parent and daughter grains is determined based upon a rotation matrix that preserves an invariant line between the parent and daughter [5]. The evolution law for the growth of the martensite phase is based on an empirical accumulated shear strain law proposed by Olson and Cohen [6]. The single crystal elastic constants for the austenite phase are as reported for 316 stainless steel [7] and the single crystal elastic constants of the martensite are taken from hardened SAE 1050 plain-carbon steel [8], see Table 1.

Table 1: Elastic constants used in the EVPSC calculations.

Material	C_{11} [GPa]	C_{12} [GPa]	C_{44} [GPa]	$2C_{44}/(C_{11}-C_{12})$
Austenite	206	133	119	3.26
Martensite	267.9	110.8	78.9	1.00

Using the simple Voce hardening law [1] the macroscopic true stress strain calculated using the EPSC model are easily fit to the measured macroscopic data, see [1]. In the calculations <110>{111} slip systems were used for the austenite and the martensite was assumed to be fully elastic. The Voce hardening parameters for the austenite used to fit the model predictions to the measured macroscopic behavior are listed in Table 2.

Table 2: Voce hardening parameters for the EVPSC model calculations

Material	τ_0 [MPa]	τ_1 [MPa]	θ_0 [MPa]	θ_1 [MPa]
Non-transforming	77	68	370	140
Transforming	60	40	2000	190

A set of 5,000 randomly oriented grains were used for each phase in the calculations. For the transforming material an initial martensite phase fraction of 0.4% was used, based upon the measured phase fractions from the diffraction measurements. Hence 10,000 grains were initially in the model, which increased to 15,000 grains as all the 5,000 austenite parent grains created a martensite daughter grain. The initial grain sets for the two phases were not the same, and thus there were no orientation relationship between the two initial grain populations, but the orientation of the daughter grains were determined from the parent orientations as described in [1].

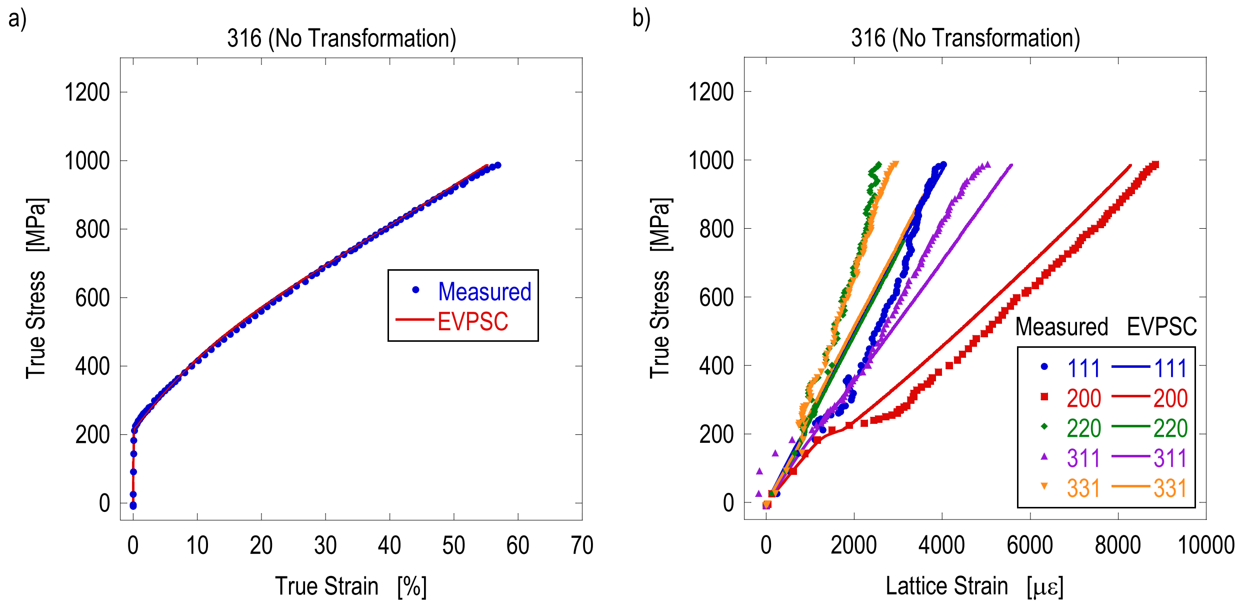

Figure 1: Measured and simulated macroscopic stress strain curve (a) and lattice strain curves (b) for the non-transforming stainless steel.

From Figure 1 it is obvious that the macroscopic behavior of the 316 stainless steel can be predicted by the EVPSC model with great accuracy. However, looking at the lattice strains the observed plastic anisotropy in the measured data is larger than the model predictions. The order of the reflections and the direction of the inflections in the elastic-plastic transition region are correctly predicted, but the spread in the plastic region is simply too low. There are not many points in the elastic region, but it looks like the elastic anisotropy is well captured by the EVPSC model.

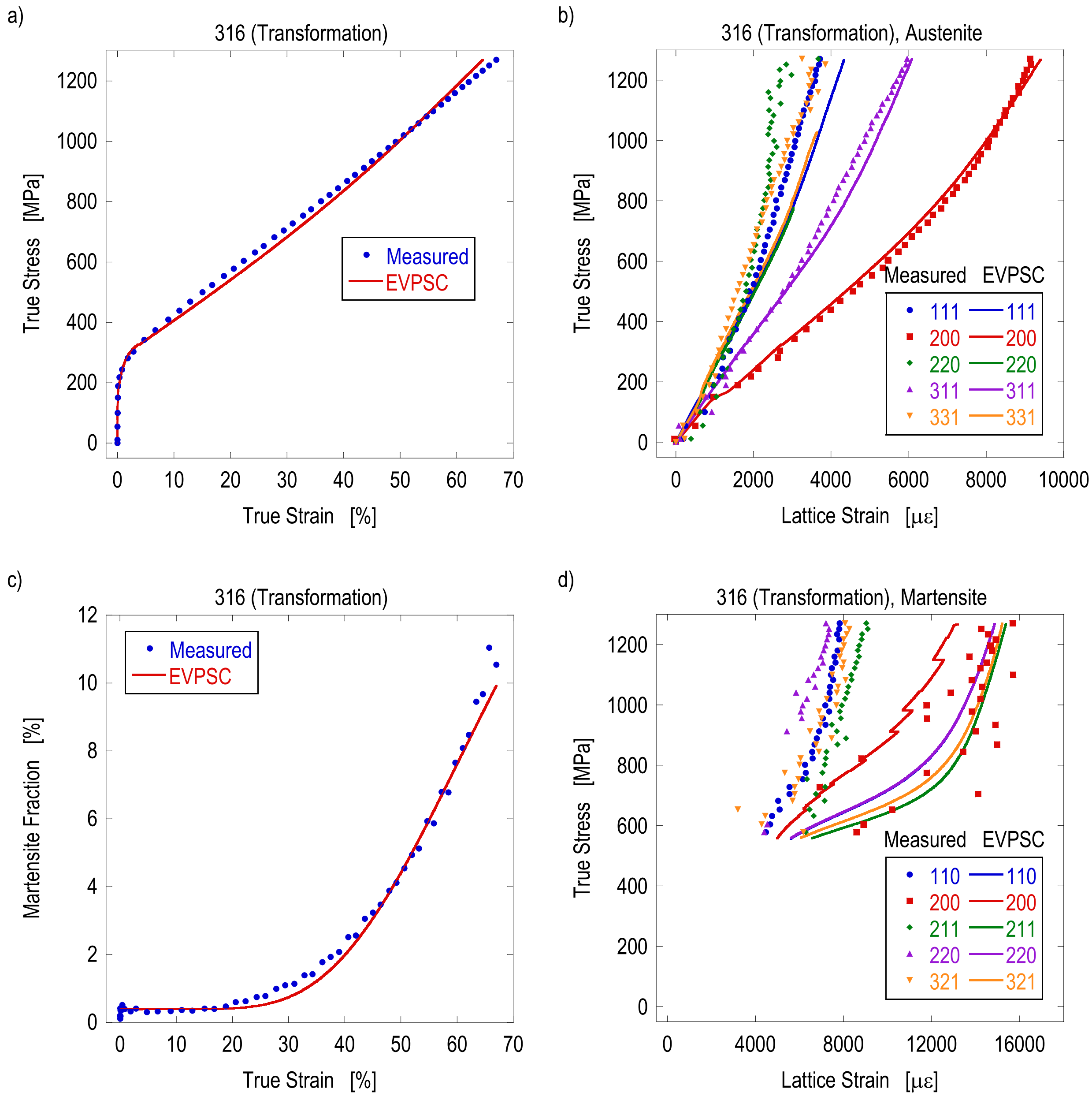

Figure 2: Measured and simulated macroscopic stress strain curve a), lattice strain curves b) and d), and martensite phase fraction c) for the phase transforming stainless steel. Notice the larger lattice strain scale in d).

From Figure 2 it is clear that the EVPSC model is able to predict the macroscopic stress strain curve and the phase evolution of the transforming stainless steel with good accuracy. The lattice strains for the austenite is also well predicted, with a bit of difference on the plastically stiff reflections (111, 220 and 331) for larger strains where the model under predict the anisotropy, but not as significant as for the non-transforming steel where the disparity gets larger with increasing stress. The martensite lattice strains are predicted to be larger than the measured (up to a factor of two), except for the 200 reflection which show significant scatter in the measurements. This could be caused by several assumptions made in the model development, including variant selection, the determination of the initial stress state in a newly formed martensite volume, phase evolution law or the martensitic phase transformation strain.

The agreement between the model predictions and the measured data is about on par with what have been shown in the literature [1,2,9], i.e. the general trends are well represented, but a quantitative lattice strain agreements is not obtained for all reflections over all stress/strain ranges. Particularly the predictions for the martensite strains are in poorer agreement due to the additional assumptions made regarding the initial state and evolution of the martensite daughter grains.

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